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Mathematical Studies of Wavelet Inverse
Reconstructions for Nondestructive Evaluation
Novel Dielectrics and Dispersion from
Chaotic Motions in Water

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1. OBJECTIVES:

The goals of this project were to perform and publish mathematical research on wavelet signal processing, periodic composite dielectrics, and to complete some work on the dispersion of water from a previous AFOSR grant. The wavelet studies were directed toward nondestructive evaluation using ultrasonic waves. The novel dielectrics were mainly the PBGS, photonic band gap structures - periodic arrays of a dielectric with permittivity ϵ_a embedded in a background dielectric with permittivity ϵ_b . Several types of disorder of these periodic objects were also studied.

2. STATUS OF THE EFFORT:

There are eleven publications, two submitted manuscripts, with two more in preparation from this project. There have been a number of invited talks presented, including one at Oberwolfach, Germany; a Gordon Conference in New England; a series of three 90-minute lectures in Madeira; and two 50-minute talks at special sessions of the American Mathematical Society in Iowa City and Albuquerque; as well as three talks at the annual QNDE meeting. A number of other smaller talks, colloquia, and seminars have also been given on the work done on this grant.

Two Ph.D. who worked on this project have graduated. Dr. Alan Van Nevel graduated in August, 1996 and Dr. Sankar Chakraborty in June 1997. Dr. Van Nevel, who was also supported by a companion AASERTS grant, received an American Society for Engineering Education Fellowship at the Naval Weapons Laboratory in China Lake, CA upon graduating and is now a member of their scientific staff. Dr. Chakraborty joined the Positron Emission Tomography group at Washington University in St. Louis MO as a Postdoctoral Fellow in Medical Physics. He is now a Postdoctoral Fellow in the Radiology Department of the Harvard Medical School. The education of two highly qualified Ph.D.'s is an important accomplishment on this grant. A Postdoctoral Fellow at Missouri, Dr. Sarah John, was also

partly supported by this grant, and has grown and developed during these three years. She has really come into her own. Her research is a big part of this project, as will be shown later in this report.

Several follow-on projects were identified for possible future study.

3. ACCOMPLISHMENTS:

The work on this grant has produced several discoveries, two new Ph.D.'s and has supported and strengthened a very strong, young Postdoctoral Fellow. The numbers $[A]$, $\{A = 1, 2, \dots, 15\}$ denote the publications, submitted manuscripts, and manuscripts in progress listed in the PUBLICATIONS section of this report. The work on this proposal was enhanced by a Research Leave from Missouri University to spend the academic year 1997-98 with the Department of Mathematics at Texas A & M University. This competitive leave provides a full salary for two semesters of research. Conversations and consultation with Professors Battle, Dobson, Narcowich, Larson and others have been educational and fun.

The first task of this project was to read and correct the proofs of papers [1-3]. Then, Chakraborty and I had the idea for the generalization of the statistical mechanics of the permittivity of water to aqueous biomolecular solutions [6] which was worked out and published.

One interesting discovery in this paper was a dielectric hysteresis effect in aqueous solutions of hemoglobin in the microwave frequency range. Glycine and myoglobin solutions did not show any such effect.

During this time, H.Kaiser's research group had some interesting questions about neutron optics which led to paper [4] and later to paper [8]. In [8] a full wavelet analysis of the neutron scattering data of a layered metallic composite was published. Reference [9] is one of my best papers. It extends and generalizes a number

of results on the so-called "Feynman path integral" for the time evolution

$$x(t) = [\exp(-tA)](x(0)) \quad (1)$$

of a solution x where A is an anti-self-adjoint infinitesimal generator of time translations. The operator A is the sum of two or more non-commuting, possibly time-dependent operators. Some results were obtained for non-linear and for spatially non-local parts of A . Theorems were given which prove the existence and uniqueness of solutions to a broader class of these evolution solutions than was previously known. Explicit formulae were given for a number of realistic cases, which do not seem to have been known. A number of combinatorial formulas were derived in this work using the generalized Baker-Campbell-Hausdorff equations which we found.

In Van Nevel's dissertation studies [5,7,12] and in our recent continuations [8], the behavior of the wavelet scale variable was investigated for ultrasonic backscatter for nondestructive evaluation. The scale is the "new" structure that wavelets have which Fourier signal processing lacks. The change from one scale to another corresponds to zooming in or out in size. The initial idea was that the features one seeks in the data are zeroes, maxima and minima. Thus, one may need small coefficients in some scales to accurately determine these features. One would expect high frequency scales for fine details, so the following empirical procedure was tested with hundreds of time traces provided by Prof. Steven Neal of the Department of Mechanical and Aerospace Engineering at Missouri University. The scales present in these ultrasound scans were 0-8 (256 data), or 0-9 (512 data in a scan) for $p = 2$ wavelets where $j = 0$ to 8 or 0 to 9 in the scale 2. The scales which were left unchanged were called exceptional scales and the rest were called ordinary scales. A threshold, ϵ which depended only on the signal-to-noise ratio was easily found. The best choice of exceptional scales were found to be $j = 3, 4, 5$. This was unexpected, so it was checked again and again. The additional study served to confirm this choice. Another study was undertaken to see if there was a "best" wavelet with no success. It was found that CN, DSN, DN wavelets with a lot of smoothness

tended to perform better; ie. $N \gg 1$ (10-28). This was interesting, and we hope will prove useful, but is not a satisfactory physical theory. Why these scales and not others? The Shannon information was studied, but failed to improve simple suboptimal Wiener filtered reconstructions of backscattered amplitudes. Some estimates by D. L. Donoho and co-workers failed even worse in their performance. This experience pointed us in the right direction. The Shannon information proved to be largely redundant with the energy error norm, that is, it added no new information. This would explain why the Shannon information added so little to the inversions. The Donoho *et al* approach used none of the information on ultrasonic scattering which has been built up in the past 20-25 years. This gave us the idea to try the Kullback-Liebler information I_{KL} . Let P be a probability distribution made from Wiener filter reconstructed scattering amplitudes, where $p_i \in P$ is the real or imaginary part of the backscattered signal. Let Q be a reference probability distribution $q_i \in Q$ where q_i is a real or imaginary part of a calculated ultrasound backscattered signal. The Kullback-Liebler information in bits is given by

$$I = - \sum p_i \log [p_i/q_i]. \quad (2)$$

Dr. Van Nevel expanded p_i 's and q_i 's in wavelet coefficients and maximized I_{KL} wavelet scales j and translations k . This turned out to leave most of the small coefficients in the scales $j = 3, 4, 5$ and improved the Wiener filter markedly. For example, the (real, imaginary) l^2 error norm were decreased from (0.8692, 1.2415) to (0.1723, 0.2513) for the C18 wavelet family! The values of j and k with large and/or exceptional wavelet scales form an information : energy island in the wavelet phase space. This method removed much of the noise from the reconstructions.

Several other methods were studied. Both a Monte Carlo method and a simulated annealing method were found by Van Nevel to perform comparably to the empirical scale choice and the Kullback-Liebler information maximization. They are non-trivial, but require much more computer time to apply. Although it is reassuring to see that all of these methods leave many of the small coefficients in scales $j = 3, 4, 5$; the only explanation which has been found so

far is the Kullback-Liebler information. This justifies the intuition in the original proposal that the total inverse reconstruction minimizes the l^2 error in the scattered energy or pressure and the information jointly, subject to the constraint of keeping the energy at the level indicated by the SNR estimate. The only information required is the approximate SNR and a known threshold, ε_T .

Dr. John published a long paper [11] which used dilations of a lattice to completely work out the sampling properties of compactly supported, orthonormal wavelets. The fact that lower N wavelets contain aliasing errors was known, but not to what extent. John worked this out in full detail. She proved that only the D wavelet satisfies the Shannon sampling rate. This Shannon wavelet is not compactly supported because it has $x \rightarrow \infty$. Dr. John also found that the correct choice; $SU(2)$ group structure of the filters rules out the pathological cases which Madysch pointed out. Daubechies had known of their existence according to Dr. Madysch. The half-angles of $SU(2)$ matrices zero these cases and only these, as shown in John's paper. She thus showed that they are an artifact of the wrong group choice for the filter matrices. The aliasing argument in this paper partially explains why higher N -wavelets perform better in our reconstructions. Besides their finer detail from additional smoothness, they also have smaller aliasing errors.

The two or more component dielectrics, or *photonic crystals* are a new class of materials whose *light* or *optical* properties can be designed and controlled. This basic knowledge will make new, fast devices for switches, high Q -tuning, filters, communication, and computation. The bandgap completely suppresses all noise whose wavevector or energy, k or E , are in the forbidden gap. This fact is physically rigorous because the noise is electromagnetic radiation emitted from atoms. Photonic crystals change the environment of the atom, which shifts their energy levels and makes certain frequency regions of noise impossible because they correspond to non-existent solutions.

The Photonic Band Structure project is going full steam, thanks to the energetic work of Sankar Chakraborty [10, 13, 15]. Regular

consultation with Prof. A. Figotin (an AFOSR/NM contractor from the University of North Carolina-Charlotte Math Department) continue to be valuable to this project. A beautiful paper by Figotin on the spectral theory of PBGS showed the PI how limited the theoretical physicists is on this subject. Figotin's theorem that two-component dielectrics with *space-filling structures at high dielectric contrast*, i.e, squares in square lattices at high dielectric contrasts maximize the band gap is a major landmark in PBGS. Unfortunately his group and ours are the only ones using this fundamental structural feature. Part of our long term agenda is to show engineers, device technologists, and theoretical physicists how useful these analytic results are in practice. For example, the abstract proof in scaled space-filling structure is greater than a corresponding non-space-filling case, but it cannot show how much because the model is quite complicated. If it is small, $<1\%$, then it is not of practical consequence. We have shown that it is $\geq 10\%$, which is quite significant. There is much more to learn on this subject, including localized defects and localization.

Chakraborty and the PI have three ways to solve the matrix discretizations of Maxwell's equations the the two periodic dielectric regions: plane waves; exact solutions for small, square lattices; and variational methods using trial functions made of linear combinations of spherical or cylindrical Mie scattering vector spherical harmonics. The plane wave solutions are most versatile for large systems containing many periodic scatterers. The exact solutions are complementary to plane waves, as they are only useful for small numbers of scatterers and are limited in the number of scattering shapes which can be solved exactly. The exact solutions have also been used for checking the accuracy of other approximations. The variational method is useful for two of the shapes which cannot be exactly solved. They have the desirable feature that $\omega(\text{var}) > \omega(\text{exact})$ but quickly lose accuracy as one goes to higher frequencies than the first ten bands.

All possible symmetric scatterer shapes have been calculated in all 2D lattices. The 3D FCC lattice has been solved. It is interesting that the theoretical physics literature contains only

plane wave calculations at a few filling factors f for a few pairs of dielectrics. (ϵ ϵ) mainly GaAs, Ge, Si which are high technology-device materials. Most authors claim 2-3% accuracy and some show 12-15 bands, yet different authors differ by $\pm(15-20)\%$ from one another for the same PBGS! The internal fields $D(\mathbf{r})$ and the density of states have been calculated and a number of new discoveries have been made. Some work on elastic waves, filters and oscillators have also been completed, while others are in progress. These are relegated to the next section.

Since the PI has studied elastic wave propagation for over 20 years for NDE studies, we formulated the PDE's for some 2-D periodic elastic composites. These devices have forbidden band gaps (stop bands), localized defects, and, possibly, localization phenomena for elastic waves.

We seem to be the only people studying biological materials in PBGS. In the microwave frequency window these systems have strong dispersion and attenuation (dissipation) which provide new physical effects. One of these is the opening of a frequency gap in the dispersion spectrum of a 3D FCC lattice. Another is the strong spatial dispersion in the attenuation $\alpha(\omega, \mathbf{k})$. The effects of wavevector lattice disorder in the response frequency and gap widths are greatly increased. However, the gap divided by the mid-gap frequency decreases as it must by a theorem of Figotin and Klein. Transmission effects and localized defects have been studied for acoustic, electromagnetic and elastic waves.

Some of the follow-on projects that directly further the mission of the Air Force include:

1. Generalized entropies and information with an understanding of the independence and redundancy of the information from the energy error norm. Study NDE to avoid "theoretical nonsense". Study real data for transient pulses.
2. Matched wavelet filters for NDE.
3. Resonant ultrasound spectroscopy inverse problem for determining the elastic stiffness constants accurately.

4. Renormalization group - wavelet analysis to tailor wavelets to problems such as PBGS, topic (2) above, and a deeper understanding of the scale variable.

4. PERSONNEL SUPPORTED:

Brian DeFacio, PI; 2 months a year for 3 years.

Sarah John, Visiting Assistant Professor; half time for 3 years.

Sankar Chakraborty, graduate student, now a Ph.D., 2 months a year for 3 years.

Stefan Gheorghiu, graduate student, 2 months a year for 2 years.

Alan Van Nevel, graduate student, now a Ph.D., (AASERTS companion grant) 2 years.

Eric Veum undergraduate, the graduate student (+ AASERTS grant), 6 months a year for one year.

Elijah Flenner, graduate student (also has AASERTS grant), 6 months a year for one year.

5. PUBLICATIONS;

1. S.- H.Kim, G.Vignale, and B.DeFacio, Dynamic Dielectric Response of Liquid Water, Phys.Rev. E 50, 4618-4624 (1994).
2. B. DeFacio, S.- H.Kim, and A.Van Nevel, "Applications of Squeezed States - Bogoliubov Transformations of the Statistical Mechanics of Water and Its Bubbles", Intl. Wkshop. on Squeezed States and Uncertainty Rel. in NASA Conf.Proc. 3270, D.Hsan, M.Rubin, Y.Shin. and M.A.Man'kov, eds., 339-351 (NASA, Greenbelt MD, 1994).
3. B.DeFacio, "Coherent-state Path Integrals and Their Relation to Wavelets" in On Klauder's Path: A Field Trip, G. G. Emch, G.Hegerfeldt, and L. Streit, eds., 43-53 (World Sci. Pubs., N.Y., NY, 1994).
4. H.Kaiser, K.Hamacher, R.Kulasekere, W.- T.Lee, J.F.Ankner, B.DeFacio, P.Miceli, and D.L.Worcester, "Neutron Inverse Optics in Layered Materials", in Inverse Optics III, M. Fiddy, ed., SPIE 2241, 78-89 (Soc. Photo. Ind. Engr., Bellingham WA, 1994).
5. D.M.Patterson and B.DeFacio, "Wavelet Inversions of Data for Elastic Wave Nondestructive Evaluation", in Inverse Optics III, M. Fiddy, ed., SPIE 2241, 172-184 (SPIE Bellingham WA, 1994).
6. S.Chakraborty and B.DeFacio, "Dynamic Frequency-Dependent Dielectric Response of Three Aqueous Biomolecular Solutions," Physica A 221, 419-437 (1995).
7. A.Van Nevel, B.DeFacio, and S.P.Neal, "An Application of Wavelet Signal Processing to Ultrasonic Nondestructive Evaluation," Rev.QNDE 15, 733-740 (1996).
8. G.Saab, B.DeFacio, H.Kaiser, and D.L.Worcester, "Wavelet Inverse Neutron Scattering Study of Layered Metallic NiC-Ti Composites," Rev.QNDE 16, 39-46 (1997).

9. B.DeFacio, G.W.Johnson, and M.Lapidus, Feynman's Operational Calculus and Evolution Equations, A.Appl.Math. 47,155-211 (1997).
10. S.Chakraborty and B.DeFacio, Periodic Composite Backing Filter for the Design of Ultrasonic Transducers, Rev.Prog.QNDE 17, 875-882 (1998).
11. S.John, Lattice Functions, Wavelet Aliasing, and $SO(3)$ Mappings of Orthonormal Filters, J. Math.Phys. 39,569-593 (1998).
12. A.J.Van Nevel, B.DeFacio, and S.P.Neal, Information-theoretic, Wavelet Noise Removal for Inverse Elastic Wave Scattering Theory, (submitted, 1998).
13. S.Chakraborty and B.DeFacio, Electromagnetic Waves in 3-D, Periodic, FCC, 2-Component Dielectric Structures Containing a Biological Material, (submitted, 1998).
14. B.DeFacio, J.A.Sjogren, and E.Flenner, The Mobius Transformation and $p=2$ Wavelets for Noisy Relaxation Processes (in preparation).
15. S.Chakraborty and B.DeFacio, High Dielectric Contrast, Microwave Frequency, 2-D Photonic Band Gap Structures with Dispersion, and Possibly, Loss Tangents (in preparation).

6. INTERACTIONS/TRANSITIONS:

a. Participation/Presentations at meetings, Conferences, etc.

1.Participant in the Program Review on Computational Electromagnetism, Brooks AFB, Jan.'95,'96,'97.

2.Invited colloquium and seminar speaker at the Physics Dept.,

University of Cincinnati, spring '95.

3. Presented talks on Wavelet Inverse Scattering, Coherent States at the March meeting of the American Physical Society, Indianapolis, IN, 1995.
4. Invited speaker (3, 90-minute lectures on Wavelet Inverse problems). European Common Market Summer School, Madeira, Portugal, 1995.
5. Presented talk, was session chair at the QNDE meeting, University of Washington, Seattle, 1995.
6. Presented 2 talks at the March meeting of the American Physical Society, St. Louis, MO, 1996.
7. Invited speaker, Oberwolfach, Germany summer of 1996.
8. Invited participant, poster session, Gordon Research Conference, Kimball Union Academy, 1996.
9. Presented talk, was session chair at the QNDE meeting. Bowdoin College, ME, 1996.
10. Presented 2 papers, was session chair at the March meeting of the American Physical Society, Kansas City, MO, 1997.
11. Presented 50 min. talk at a special session of the American Math. Society on Localization and other Multiple Scattering Phenomena of Classical Waves, Albuquerque, NM, 1997.
12. "Radial Basis Functions for Elastic Wave Inverse Theory" at the Center for Approximation Theory, "PBGS" at Condensed Matter Seminar, "I., Information Theory for Wavelet Inverse Problems" and "II., Information Theory for Elastic Waves", at the Atomic & Laser Physics Seminar, Texas A & M University, College Sta., TX, 1997

b. Consultative and advisory activities at laboratories, other groups, etc.

1. Prof. A. Figotin, Department of Mathematics, University of North Carolina-Charlotte; Localization, photonic band gap materials.
2. Dr. C.M. Fortunko, National Institute of Standards and Technology, Materials Reliability Division, Boulder, CO. Analysis of transient pulses using wavelets error analysis at all stages. Non-linear ultrasonics and plate Green's distributions using wavelets are being studied. A more accurate experimental value of the wave propagation speed of elastic waves is under study.
3. Prof. S.P. Neal's Ultrasonic Laboratory at Missouri University in the Department of Mechanical and Aerospace Engineering. Inverse problems with ultrasound.
4. Dr. Frank Margatan, NSF NDE Center at Iowa State University. Grain noise scattering.

4. TRANSITIONS:

1. The PI, with some excellent help from Dr. Van Nevel and Mr. Eric Veum, spent several days working out answers to questions and criticism by three referees at a journal on a series of measurements by Drs. Kyle Hollman and C.M. Fortunko. They are developing new resonant methods for measuring the speed of sound more accurately than is possible today, and we intend to continue to contribute theoretical modeling and signal processing on this project.
2. Van Nevel has taken some ideas which he started developing in his dissertation here and has extended them at the Naval Weapons Center in China Lake (where he is now a member of the scientific staff). His result uses wavelet frames to detect

and classify texture in transient radar signals.

8. NEW DISCOVERIES:

A number of new discoveries have been made. The dielectric hysteresis in aqueous solutions of hemoglobin at microwave frequencies and a better model for the permittivity of water were completed (from a previous project). The effects of dispersion and dissipation in photonic band gap structures were treated and were shown to open the pseudogap in water scatterers in the microwave frequency region. Wavelet methods were developed for non-destructive evaluation of high technology materials. The wavelet scales were shown to carry large information in small coefficients and the mid-range scales $j = 3, 4, 5$ for ultrasound scattering with data populating scales $j = 0, 1, \dots, 8$ (or 9). Then the maximization of the Kullback-Liebler information was shown a similar effect. We have thus reached the conclusion that it is the Kullback-Liebler information which improves these conversions. D. John gave a complete discussion of the aliasing of compactly supported, orthonormal wavelets. She showed that it is a $SU(2)$ group for the $p = 2$ instead of the usual $U(2)$ which removed all of the pathological multiresolutions. It is the half angles in the $SSU(2)$ matrices which force the unwanted cases to vanish. Periodic arrays of Young's modulus and/or permittivity PBGS have been studied for their acoustic, electromagnetic and elastic wave frequency spectra. Lattice disorder, localized defects and transmission coefficients have been studied in these composites. A potential elastic wave filter utilizing the forbidden gaps was discovered. The University of Missouri is considering applying for a patent on this filter.

9. HONORS AND AWARDS:

Fellow of the American Physical Society

Listed in Who's Who in Science and Engineering.

International Advisory Board, J.Non-destructive Testing and Evaluation, Elsevier Publishers, Oxford University.

Research leave, 1997-98 to Texas A&M University from Missouri University.

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Adjusted Budget
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Equipment	(Computer equipment, maintenance)	\$463.48
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Travel	(meetings, research collaborations)	\$3365.58
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13. ABSTRACT (Maximum 200 words) Wavelet inverse methods for non-destructive evaluation of high technology materials using transient pulses of ultrasound have been developed using the Kullback-Liebler information. This selects scales with small energy wavelet coefficients which have large information content. Wavelet aliasing by all compactly supported orthonormal wavelet families has been proven, and pathological multiresolutions were ruled out by choosing the correct group for the filters, $SU(2)$. The PBGS, photonic band gap structures, have been studied for electromagnetic and elastic waves. These periodic, two-component dielectrics have been studied with loss-tangent (dissipation) dispersion and lattice-disorder. Localized defects have been studied. An elastic wave filter and a gap opened by the high contrast of water at microwave frequencies were found.					
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